Electron Diffraction on Boron Nitride Nanotubes

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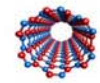
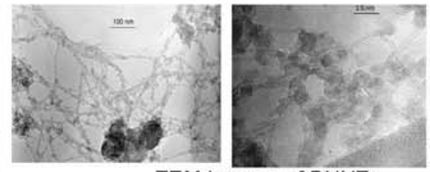
Motivation

Boron nitride nanotubes (**BNNTs**) show an insulating character with a constant band gap (> 5.5 eV) which make them a possible alternative to their carbon brethren in regards to possible applications.

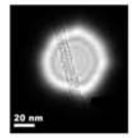
Detailed knowledge of the atomic structure of BNNTs (chiral angle and diameter) is still wanting despite the fact that this is key to understanding their **growth mechanism** which is necessary to control their formation and to improve their yield.

Nano beam electron diffraction is the best mode to develop this work because it allows a high coherent and parallel nanometer-sized electron beam.





TEM images of BNNTs



Bright field image of a BNNT

Results

At the expense of replacing a carbon-carbon pair by a B-N one, BNNTs and CNT share the same structures, which can be described by the set of the two **chiral indices** (n,m) or equivalently a **diameter d** and an **helicity θ**.

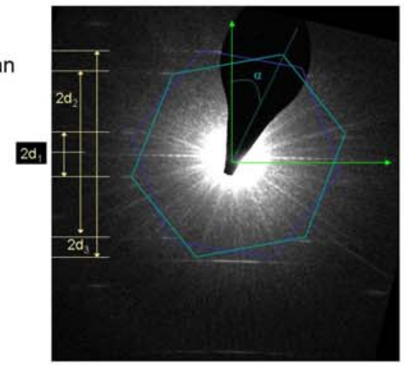
<u>Electron diffraction patterns (**EDP**) of a **single-walled BNNT**:</u>

Layer-lines are perpendicular to the tube axis direction and the central line is called the **equatorial line** (Eq-L).

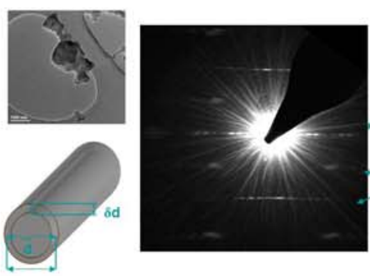
The **helicity** (α) of a NT is deduced by measuring the ratio of the layer lines distances. α (Fig.) = 18.7 deg.

$$\alpha = \text{arctg}\left[\frac{2\,d_2 - d_3}{d_3\sqrt{3}}\right]$$

The tube **diameter** can be extracted from the period of the pseudooscillations along the layers. d (Fig.) = 3.27 nm



<u>EDP of a **double-walled BNNT:**</u>



Eq. Line Analysis

$\bar{d}$ = 1.846 ± 0.09 nm

δd = 0.412 ± 0.02 nm

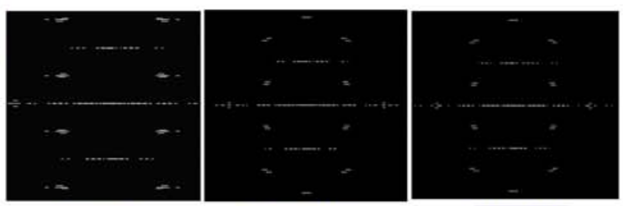
Helicity

α_A = 0.0 ± 0.02 °

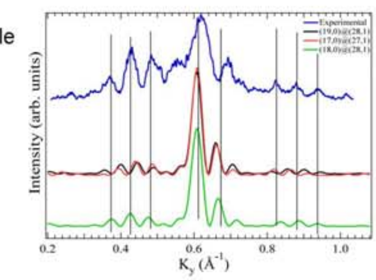
α_B = 1.96 ± 0.08 °

An EDP of a double-walled (DW) can be interpreted as the simple superposition of the layer-lines of the two constituent tubes.

This DW-BNNT is composed of **(18,0)@(28,1)** tubes.

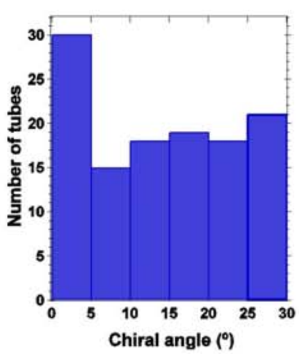


(18,0)@(28,1) (17,0)@(27,1) (19,0)@(28,1)



Profile of the 3rd layer-line for the experimental and simulated EDP of the DWNT

Impact



Chiral angle distribution extracted of the EDP analysis

We have acquired the **first** EDP of individual **single-walled** (SW) BNNTs and ropes of BNNTs.

We have measured the **chiral angles** of 121 **BNNTs** (including SW, multi-walled and ropes of BNNTs) and **diameters** of 26 of those NTs.

Comparing with the simulated EDP obtained using the kinematical theory of diffraction, we determined, for the first time, the **chiral indices** of SW and double-walled BNNTs.

The analysis of the EDP of these BNNTs revealed to us that **12 %** of the BNNTs are **zig-zag**, while the distribution of the other helicities is uniform. These studies led to a deeper understanding of the formation mechanism of he tubes, because this preferential zig-zag helicity of the tubes is likely related to their **catalytic growth**.

Future directions

The future applications of these materials require huge quantities of long NTs. The use of ropes of NTs could solve both points. We will focus then, in the analysis of the EDP of these ropes of BNNTs. Due to the structural configuration of these objects, this kind of analysis is more complex that for single-walled and double-walled BNNTs. Nevertheless this information is very important to enable a better understanding of their growth and of the interactions between the BN networks.

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